Slow manifold Boris algorithm for particle simulation and study of AE frequency chirping using M3D-C1

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Overview

1. Implementation of slow manifold Boris algorithm in M3D-C1

2. Study of Alfven eigenmode frequency chirping

Implementation of slow manifold Boris algorithm in M3D-C1

Introduction to M3D-C1 kinetic module

- M3D-C1 is an upgrade and rewrite of the M3D MHD code. With more advanced finite-element representation and implicit time advance method, M3D-C1 can study the nonlinear problem with larger timestep and save computation time.
    - MHD equations are evolved using implicit or semi-implicit method.
- We want to have the same capability of the kinetic module of M3D-K code in M3D-C1, to study the interaction between energetic ions and MHD activities (Alfvén waves, kink/tearing modes etc).
    - Explicit particle pushing can be accelerated using modern HPC with GPU, like in PIC codes.

Particle pushing based on guiding-center model

$$\frac{d\mathbf{X}}{dt} = \frac{1}{B^*}\left(v_\parallel \mathbf{B}^* - \mathbf{b} \times \mathbf{E}^*\right)$$

$$m\frac{d\mathbf{v}_\parallel}{dt} = \frac{q}{B^*}\mathbf{B}^* \cdot \mathbf{E}^*$$

$$\mathbf{B}^* = \mathbf{B} + \frac{mv_\parallel}{e}\nabla \times \mathbf{b}, \qquad B^* = \mathbf{B}^* \cdot \mathbf{b}$$

$$\mathbf{E}^* = \mathbf{E} - \frac{mv_\parallel}{e}\frac{\partial \mathbf{b}}{\partial t} - \frac{\mu}{q}\nabla B$$

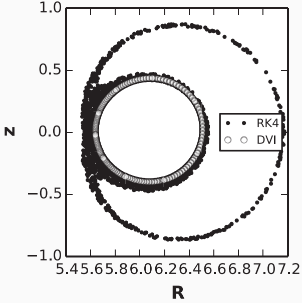
- Particle markers are advanced using 4th order Runge-Kutta.

Coupling particle and MHD simulations

- Kinetic effects are coupled into MHD equation through pressure coupling or current coupling.
- The MHD field information is uploaded to GPU memory at the end of MHD timestep, and particles are pushed on GPU.
- The particles data is downloaded from GPU and used for pressure or current calculation.
- We use subcycles for particle pushing to reduce GPU-CPU communications.
    - Fields are fixed during subcycles, which can lead to some error for particle pushing calculation.

Review of previous work on conservative method for particle pushing

- Particle pushing based on Runge-Kutta method suffers from accumulation of numerical error and can lead to nonphysical results for long-time simulation.
- Simplectic integrator possess conserved quantities in the simulation, thus can be used to simulate long-time evolution of a dynamic system.
    - For simple Hamiltonian system, simplectic integrators can be easily constructed and have shown excellent conservation properties.
- For guiding-center system, the integrator is difficult to construct and the result algorithm is often implicit. In addition, the method can suffer from "parasite mode" which can lead to numerical instabilities.
- One can construct a degenerate variational integrator (DVI) to get rid of parasite mode, but this requires limitations on the form of magnetic fields.

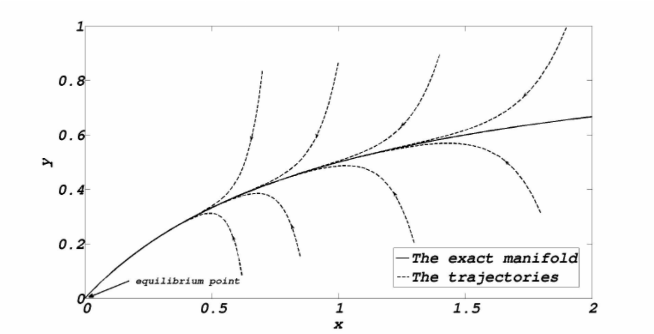


H. Qin and X. Guan, Phys. Rev. Lett. 100, 035006 (2008).
C.L. Ellison, J.M. Finn, J.W. Burby, M. Kraus, H. Qin, and W.M. Tang, Phys. Plasmas 25, 052502 (2018).

Slow manifold can be used to simplify multi timescale problem

- Slow manifold characterizes the equilibrium point of fast motion, which can be used to reduce the dimension of dynamical system.
- For system with motions of multiple timescale, slow manifold gives a solution of the equation of motion, where the fast motion is absent.

$$\begin{aligned} \epsilon\dot{y} &= f_\epsilon(x,y) \quad &\rightarrow \quad 0 &= f_0(x,y) \\ \dot{x} &= g_\epsilon(x,y) \quad & \dot{x} &= g_0(x,y) \end{aligned}$$



J.W. Burby, Journal of Mathematical Physics 61, 012703 (2020).

Slow manifold + Boris provides a structure preserving algorithm for particle motion

- For particle motion in the magnetic field, slow manifold is the set of special particle trajectories where gyro motion is absent, and only parallel motion and drift motion is present.
- For these trajectories, there is only one timescale. One can use the full-orbit particle pushing algorithm to calculate the trajectory with large time-step.
    - This requires the numerical method to be stable, like implicit method.
    - Boris algorithm is a good candidate that is stable (implicit) and structure preserving.
- The effect of gyro motion on the slow motion can be calculated by including an effective electric force $-\mu\nabla B$.

J. Xiao and H. Qin, ArXiv:2006.03818 (2020).

Tips for implementing Boris slow-manifold algorithm

- Boris algorithm is similar to a leap-frog method where x and v are evolved at interleaved time points.
    - We should use a Cartesian coordinate to avoid coordinate transformation in dx/dt.
    - When calculating the energy and toroidal momentum, x and v at the same time should be used.

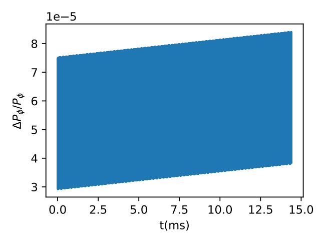
$$
\begin{aligned}
x_{l+1} &= x_l + v_{l+1/2}\Delta t \\
v_{l+3/2} &= v_{l+1/2} + \left(E^{\dagger}_{l+1} + \frac{v_{l+3/2} + v_{l+1/2}}{2} \times B_{l+1} \right) \Delta t \\
E^{\dagger}_{l+1} &= E_{l+1} - \mu \nabla B_{l+1} \\
v_{l+1} &= (v_{l+3/2} + v_{l+1/2})/2
\end{aligned}
$$

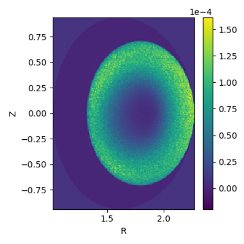
- Particles should be initialized carefully to stay on the slow manifold, which includes all the drift terms.

Conservation of toroidal momentum

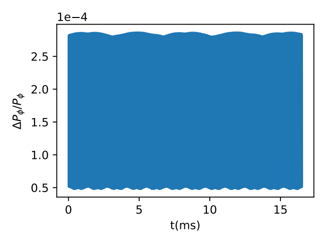
$B = 2\text{T}$, $E = 130\text{keV}$ ($v = 5 \times 10^6 \text{m/s}$), $dt = 6.5 \times 10^{-8}\text{s} = 2\pi/\Omega$

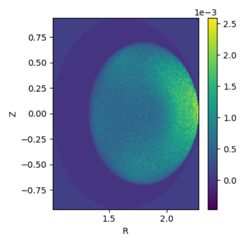
Guiding center RK4:





Boris:

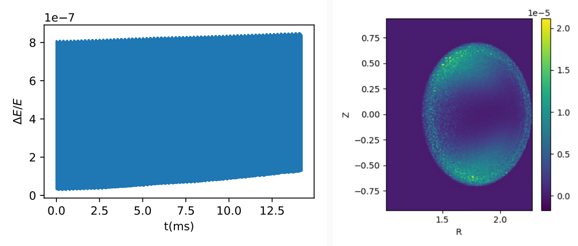




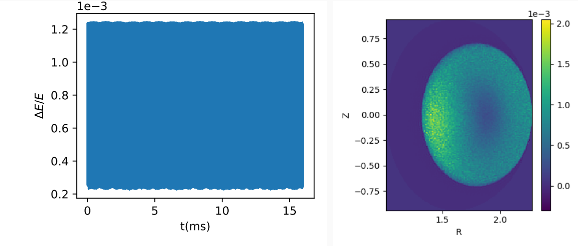
Conservation of kinetic energy

$B = 2\text{T}$, $E = 130\text{keV}$ ($v = 5 \times 10^6 \text{m/s}$), $dt = 6.5 \times 10^{-8}\text{s} = 2\pi/\Omega$

Guiding center RK4:

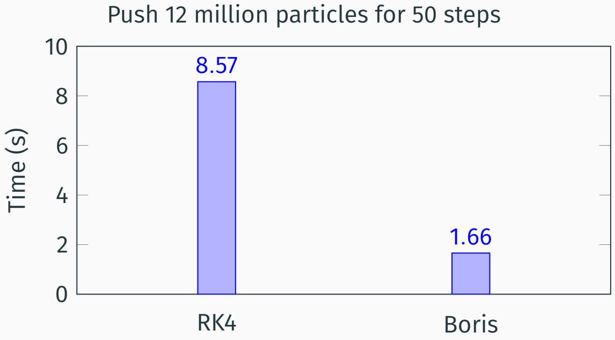


Boris:



Advantages of slow manifold Boris algorithm

- The conservation properties of both RK4 and Boris are both good enough for 10ms simulation.
- However, the benefits of Boris is that the calculation is much simpler than RK4 for each timestep.
  - One only needs to do one time of field calculation instead of 4 times.
  - There is no need to calculate curvature term ($\nabla \times \mathbf{b}$), and the mirror force ($-\mu\nabla B$) can be treated as a gradient of scalar.
- The speedup can be more attractive by using a larger timestep for Boris.



Shortcomings

- Instead of 5D, we now need to store 7D information of particles (3X+3V+μ).
- The conservation law of P_ϕ and E is not as good as RK4.
    - Try a higher order method of Boris.
    - Use a different structure-preserving algorithm than Boris to evolve x and v at the same timestep like in RK4

Application in runaway electrons?

- The long-time conservation property of algorithm is more important for runaway electron simulations.
- If we can show that Boris works for RE, it can be beneficial for tokamak disruption simulations
  - RE is acclerated by parallel electric field mainly, so we can assume $\mu = 0$ and ignore the mirror force term.
  - It is a question of whether μ can be treated as an adiabetic invariant or not.
  - Extend the classical Boris algorithm to relativistic particles

Study of Alfven eigenmode frequency chirping

Frequency chirping of Alfven eigenmodes

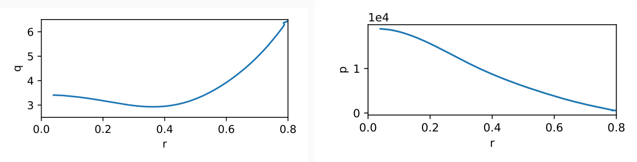
- Frequency chirping is widely observed in AEs excited by EPs in tokamaks.
- Berk-Breizman theory gives a solid explanation about up and down frequency chirping through clump-hole formation.
- It is computationally expensive to do a full nonlinear simulation for both particles and MHD field for a long time (>10ms$\sim 10^4\tau_A$)

Semi-linear method for particle-MHD simulation

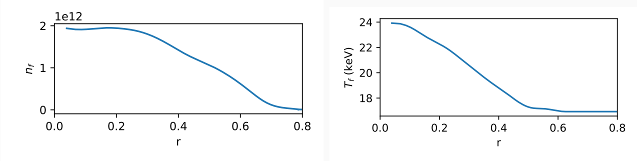
- Recently Roscoe White presented his study on mode frequency chirping using ORBIT, which utilized NOVA to calculate the eigenmode structure, and information from ORBIT particles to calculate mode amplitude and phase changes using δf method.
    - This study shows that the frequency chirping is caused by nonlinear effects in particles instead that in MHD modes.
- To study the frequency chirping, one can do a linear MHD simulation plus a nonlinear particle simulation.
    - There is only one mode get excited, and mode-mode interaction is not important.
    - The mode saturation and frequency chirping is due to the flattening of particle distribution function and clump-hole formation, which can be incorporated through a nonlinear δf method.
- For M3D-C1, linear MHD equations are much easier to simulate since there is no need to calculate and factorize MHD equation matrix at every timestep.
    - The particle simulation is also easier to do since the basis function is easier to calculation for 2D mesh than 3D.

Use a DIII-D equalibrium to study excitation of RSAE

- $B_0 = 2\text{T}$, $R = 1.6435\text{m}$, $a = 0.627\text{m}$
- q profile has a mininum at with $q_{min} = 2.93$ at $r = 0.36\text{m}$



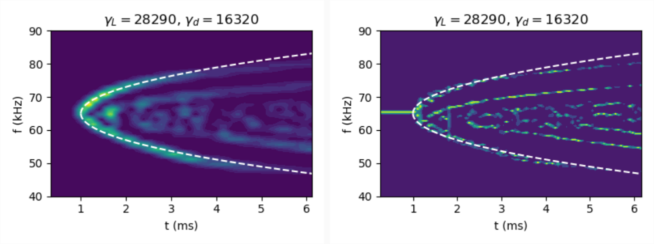
- EP follows a Maxellian distribution in momentum space.



S. Taimourzadeh et al., Nucl. Fusion 59, 066006 (2019)

Spectrogram analysis using DMUSIC

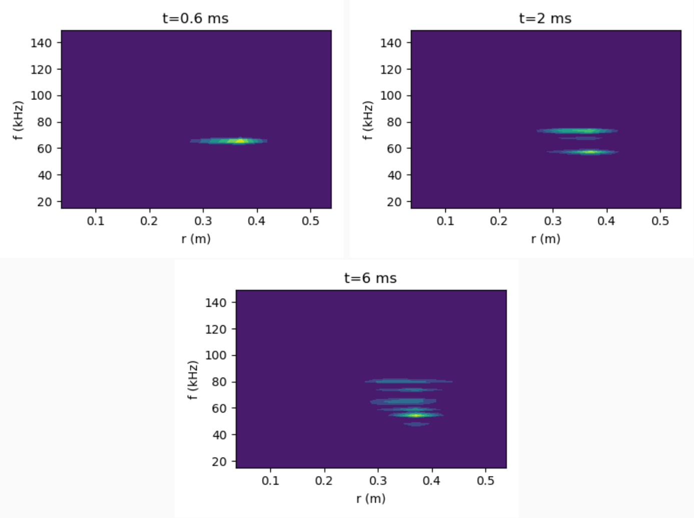
- DMUSIC is an algorithm used for frequency detection by performing an eigen decomposition of the covariance matrix of signal samples.
    - By choosing the N maximum eigenvalues for the correlation matrix, we can separate the signal subspace and the noise subspace, and then use the orthogonality between two subspaces to calculate the characteristic frequency and damping rate in the signal subspace.
    - The estimator function is strongly peaked at the signal frequency, which can give a sharper result than FFT spectrogram.



- The result shows that frequency chirping rate is consistent with the Berk-Breizman theory.

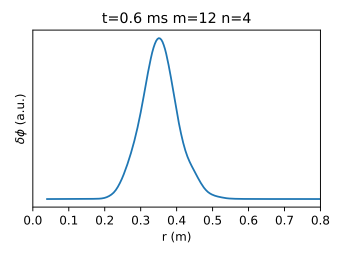
$$\delta f = \frac{16\sqrt{2}}{\pi^2 3\sqrt{3}} \gamma_L \sqrt{\gamma_d t}$$

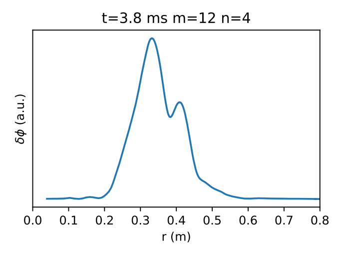
Mode structure

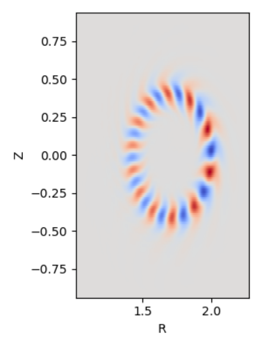


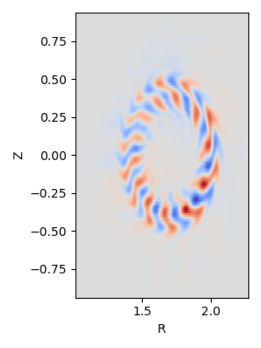
- The mode structure of the modes after splitting are not identical. The high frequency branch has a broader radial distribution.

Mode structure

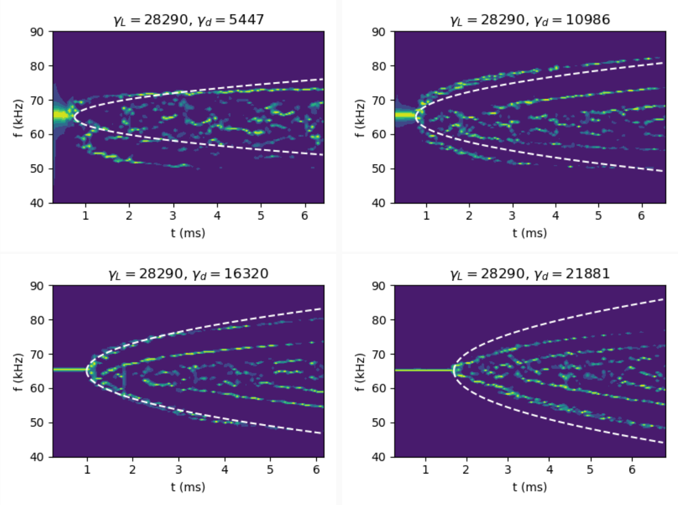






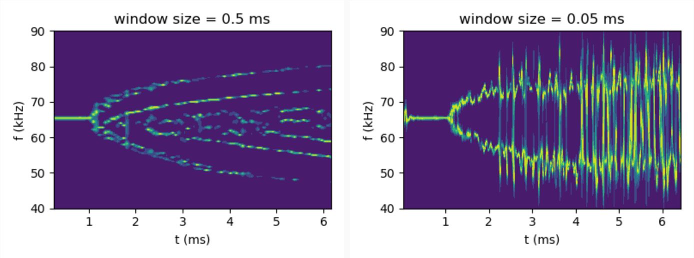


Frequency chirping for marginal and unmarginal cases



- The chirping rate is consistent with Berk-Breizman chirping rate for unmarginal case, but for marginal case ($\gamma_d \sim \gamma$), the chirping rate is smaller than the theory predicts.

Using different time window to analyze chirping at different timescales



- By using a smaller time window in DMUSIC analysis, we can analyze the fast chirping behavior for each frequency band.
  - This may be caused by particle motion which has a smaller timescale.

Summary and future work

- Slow manifold Boris algorithm can help particle simulation use large timestep and simplify requirement of field calculation, while improve long time conservation property.
- Frequency chirping of AEs can be simulated by combining a linear MHD simulation with a nonlinear particle simulation, which can save computation time and gives a reasonable result.
- The structures of up and down chirping modes are different, which can lead to asymmetric chirping observed in experiments.
- Future work:
  - Do nonlinear MHD simulation to benchmark with this semi-linear method.
  - Try to understand the discrepancy of chirping rate between theory and simulation for the marginal case.
  - Use this semi-linear method to study Alfven wave avalanche with multiple modes excitation and chirping.